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NCASI ENHANCEMENTS OF QUAL-II MODEL

by

Linfield C. Brown, Raymond C. Whittemore*,
and Thomas O. Barnwell, Jr.**

Department of Civil Engineering
Tufts University
Medford, MA 02155

*Northeast Regional Center
National Council for Air and Stream Improvement
Tufts University
Medford, MA 02155

**Environmental Research Laboratory
U.S. Environmental Protection Agency
Athens, GA 30613

ENVIRONMENTAL RESEARCH LABORATORY
OFFICE OF RESEARCH AND DEVELOPMENT
U.S. ENVIRONMENTAL PROTECTION AGENCY
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16. ABSTRACT

The mathematical water quality model QUAL-II was modified to reflect advances in the understanding of algal, nutrient, and light interactions. Code changes also were made to incorporate hydraulic, boundary condition, water quality constituent, and rate coefficient features that had utility in other steady state water quality models. The new model provides an increased number of simulation options and a comprehensive output format designed to aid in calibration and verification.

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NCASI Enhancements of the QUAL-II Model

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Linfield C. Brown[a], Raymond C. Whittemore[b], and Thomas O. Barnwell[c]

1.0 Introduction

The mathematical water quality model QUAL-II has been modified to reflect advances in the understanding of algal, nutrient, and light interactions. Code changes were also made to incorporate hydraulic, boundary condition, water quality constituent, and rate coefficient features that had utility in other steady state water quality models. The new model provides an increased number of simulation options and a comprehensive output format designed to aid in calibration and verification.

Specific changes and additions to the model code are outlined in Table 1. A schematic diagram of water quality constituent interactions is shown in Figure 1. Most of these features were adapted from versions of QUAL-II currently in the public domain, including those attributed to the Texas Water Development Board (13), the Southeast Michigan Council of Governments (11), and Meta Systems (6). The new model version has the acronym QUAL2E. The work was performed by NCASI with partial funding from the EPA Center for Water Quality Modeling (CWQM), Athens, GA. The new code is part of the CWQM model library and is supported and distributed to users as the "standard" QUAL-II code.

2.0 Impetus For This Project

As discussed in NCASI Technical Bulletin No. 391 (7), the version of the model QUAL-II documented, tested and revised by NCASI was obtained from the Southeast Michigan Council of Governments (SEMCOG). The model was originally developed by Water Resources Engineers, Inc. (now Camp, Dresser, McKee, Inc.). This version was selected by NCASI because of the availability of quality documentation (10). The revised SEMCOG version of QUAL-II has been used extensively by both consultant and regulatory personnel.

NCASI's application of the revised version of QUAL-II/SEMCOG on the Ouachita River Basin provided justification for the current reexamination of the QUAL-II model code (8). In this study, water quality simulations were examined for portions of a deep, low velocity river

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[a]Dept. of Civil Engineering, Tufts Univ., Medford, Ma 02155.

[b]Northeast Regional Center, NCASI, Tufts Univ., Medford, MA 02155.

[c]U.S. EPA, Environmental Research Laboratory, Athens, GA 30613.

where algal dynamics were dominant. Algal cells were productive in a small zone near the surface where they could expect to grow at a near optimum rate. However, QUAL-II/SEMCOG requires that the algae be productive over the entire water column under some artificially low light intensity. The light intensity calculated is that single average value necessary to achieve the same algal productivity that actually occurs over a 24 hour diurnal cycle. As the river becomes deeper, the model distributes the available light over a larger volume and produces both lower growth rates and D.O. levels. The field data showed that in these areas the model could not reasonably simulate the algal productivity required to match the high observed D.O. levels. The problem was traced to the manner in which the diurnal average light intensity was computed.

3.0 NCASI/EPA Enhancements to QUAL-II

The NCASI/EPA enhancements to the QUAL-II code are outlined in Table 1 and are discussed briefly in this paper. All of the enhancements are described in detail in the QUAL2E Documentation Report (2) and User's Manual (9). These reports also provide guidance for selection among the various simulation options.

3.1 New State Variables

3.1.1 Nitrogen cycle

In natural aerobic waters, there is a stepwise transformation from organic nitrogen to ammonia, to nitrite, and finally to nitrate. The nitrogen cycle in QUAL2E contains all of these components, as shown in Figure 1. The incorporation of organic nitrogen as a state variable, an organic nitrogen settling term, and an algal nitrogen uptake preference factor are the primary enhancements to the nitrogen cycle in QUAL2E compared to QUAL-II/SEMCOG.

3.1.2 Phosphorus cycle

The phosphorus cycle is similar to the nitrogen cycle. Organic phosphorus is generated by the death of algae and converted to the dissolved inorganic state, where it is available to algae for primary production. QUAL2E revises QUALII/SEMCOG, which included only dissolved phosphorus, to simulate the interactions between organic and dissolved phosphorus, including an organic phosphorus settling term.

3.2 Algal Growth Rate Computations

3.2.1 Algal growth rate options

The local specific growth rate of algae is known to be coupled to the availability of required nutrients (nitrogen and phosphorus) and light. QUAL2E has the capability of modeling these interactions by using three different mathematical formulations (3); a multiplicative, a limiting nutrient, or an inverse additive option.

In the multiplicative option, the kinetic expressions used to represent the effects of nitrogen, phosphorus, and light are multiplied together to determine their net effect on the local algal growth rate. This method has as its biological basis the multiplicative effects of

enzymatic processes involved in photosynthesis. The limiting nutrient option represents the local algal growth rate as limited by light and either nitrogen or phosphorus, but not both. Thus, the nutrient/light effects are multiplicative, but the nutrient/nutrient effects are alternate. This formulation mimics Liebig's law of the minimum. The inverse additive option is mathematically analogous to the total resistance of two resistors in series. In this method, an effective nutrient limitation factor is computed as the average of the inverse reciprocals of the individual nitrogen and phosphorus growth limitation factors.

3.2.2 Algal light functions

A variety of mathematical relationships between photosynthesis and light have been reported in the literature (4). Although they differ in mathematical form, all show increasing rate of photosynthesis with increasing light intensity up to a maximum or saturation value. At high light intensities some of the expressions exhibit photoinhibition.

QUAL2E recognizes three options for computing the algal growth limitation factor for light. Light attenuation effects on the algal growth rate may be simulated using a Monod half-saturation method (14), Smith's function (11), or Steele's equation (12).

Smith's function is formulated similarly to the Monod expression, but includes second order effects of light intensity. Steele's equation incorporates an exponential function to model the effect of photoinhibition on the algal growth rate. All three light function options are integrated over the depth of flow to obtain the depth averaged light attenuation factor.

3.2.3 Light averaging options (Diurnal Averaging)

Steady state algal simulations require computation of an average growth attenuation factor for light over the diurnal cycle. There are four options in QUAL2E for computing this average. The options arise from combinations of situations regarding two factors: (a) the source of the solar radiation data used in the computation, i.e., whether it is supplied externally by the user or calculated internally in the temperature heat balance; and (b) the nature of the averaging process, i.e., whether hourly values of the light attenuation factor are averaged, or a single daylight average value of solar radiation is used to estimate the mean daily value.

The selection of a light averaging option depends on the detail to which the user wishes to account for the diurnal variation in light intensity. Options 1 and 2 use a single calculation based on an "average" daily solar radiation value. Options 3 and 4 calculate hourly values of the light factor from hourly values of solar radiation and then average the hourly values to obtain the daily average value. Options 1 and 3 use the solar radiation from the temperature heat balance routines (thus both algae and temperature simulations draw on the same source for solar radiation). Options 2 and 4 use the solar radiation value provided by the user for algae simulation. A light averaging factor is used to provide similarity in calculations between options 1 and 2 versus options 3 and 4. A solar radiation factor, used only with options 1 and 3, specifies the fraction of the solar radiation computed in the heat balance which is photosynthetically active.

3.2.4 Algal self shading

In QUAL2E, the light extinction coefficient is coupled to the algal density through a nonlinear equation with user specified coefficients. Appropriate selection of these coefficients allows a variety of algal self shading relationships to be modeled, e.g., a constant extinction coefficient (non-algal turbidity) or a linear or nonlinear (Riley Equation) algal self shading effect (14).

3.2.5 Algal-nitrogen relationships

The algal growth limitation factor for nitrogen is defined by a Monod half saturation expression that uses the effective local concentration of available inorganic nitrogen, i.e., the sum of the ammonia and nitrate concentrations. QUAL-II/SEMCOG makes this calculation using the nitrate concentration only. QUAL2E allows the user to specify an algal nitrogen uptake preference factor for ammonia.

3.3 Dissolved Oxygen

The dissolved oxygen simulation in QUAL2E has been modified to include two new options and two revised computational strategies. The two new options are (a) an oxygen source/sink by reaeration of water flowing over a dam and (b) the capability of inhibiting the rate of nitrification at low dissolved oxygen concentrations. The dam reaeration option uses the method attributed to Gameson (16). The nitrification inhibition option employs a correction factor computed from a first order equation in dissolved oxygen concentration. The correction factor is applied to the ammonia and nitrite oxidation rate coefficients.

The two new computational strategies affect the dissolved oxygen saturation concentration and the sediment oxygen demand (SOD). The DO saturation values are computed from the equations in the 16th edition of Standard Methods (1) and are corrected for temperature and atmospheric pressure. The units of SOD in QUAL2E are the traditional per unit of bottom area (gm/ft^2-day or gm/m^2-day) rather than the per unit of length in QUAL-II/SEMCOG.

3.4 Temperature

The temperature values computed in QUAL2E are used to correct the rate coefficients in the source/sink terms for the other water quality variables. These coefficients are input at 20C and are then corrected to ambient temperature using a Streeter-Phelps type formulation. The values of the temperature correction factors (theta values) may be specified by the user. In the absence of user specified values, default values are employed.

3.5 Arbitrary Non-Conservative Constituent

QUAL2E has the provision for modeling an arbitrary nonconservative constituent. In addition to a first order decay mechanism, there are source (zero order) and sink (first order) terms in the mass balance.

The expanded modeling capability for this constituent may be useful in simulating toxic materials.

3.6 Hydraulics

Experience with QUAL-II/SEMCOG showed that dispersion coefficients computed from Elder's equation may be one to two orders of magnitude smaller than observed values. To correct this problem, QUAL2E uses a generalization of Elder's equation for longitudinal dispersion as proposed by Fisher (5). QUAL2E also has the enhanced capability to model incremental outflow from a reach.

3.7 Downstream Boundary

QUAL2E has the option for specifying downstream boundary water quality constituent concentrations. This feature is useful in modeling systems with large dispersion in the lower reaches. When downstream boundary concentrations are supplied, the solution generated by QUAL2E will be constrained by this boundary condition. If the concentrations are not provided, the constituent concentrations in the most downstream element will be computed in the normal fashion.

3.8 Input/Output Modifications

The output of a QUAL2E simulation has been enlarged to provide more diagnostic and graphical features. In addition to a line printer plot of DO and BOD, the output consists of a detailed summary of the hydraulic computations, the components of the dissolved oxygen mass balance, and the components of the algal growth rate calculations. Intermediate output includes an echo printing of the climatology data, a summary of the steady state convergence iterations, and a listing of the conditions for the algal growth and temperature computations. A revised set of input coding forms has been prepared and a program for converting SEMCOG input data files to QUAL2E input format is available.

4.0 Example Application

In the Ouachita River Basin study (8) NCASI demonstrated the difficulty in simulating adequate algae growth with QUAL-II/SEMCOG. The source of the problem was attributed to the manner in which the diurnally averaged algal growth rate attenuation factor for light is computed. To test whether QUAL2E had corrected this problem, the same input data set that was used to calibrate QUAL-II/SEMCOG to the Ouachita survey was applied to QUAL2E. The results showed that the algae simulation was much improved. Where QUAL-II/SEMCOG forecast DO values of 0.5-3.0 mg/L, QUAL2E predicted values of 7.5-11.5 mg/L. In addition, chlorophyll *a* values increased by a factor of 6 to 8.

To achieve an adequate DO calibration with QUAL-II/SEMCOG, NCASI had to adjust most of the input algae coefficients to the extreme end of their suggested range of values. In addition, measured values of the light extinction coefficient and the intensity of solar radiation were adjusted to the extremes of their confidence intervals in order to force the model to produce algal growth. With QUAL2E, however, all of the algae coefficients could be placed near their expected or mid-range values to produce an adequate DO simulation.

5.0 Summary

The QUAL-II/SEMCOG model has been modified to correct errors in the computation of the algal growth rate attenuation factor for light. The code has been enhanced to reflect other algal-nutrient interactions, as well as a variety of hydraulic, dissolved oxygen, and rate coefficient features (Table 1). The success and utility of these changes has been demonstrated by application to NCASI survey data from the Ouachita River. The calibration/verification difficulties encountered with QUAL-II/SEMCOG in that study were alleviated using QUAL2E. The QUAL2E model is supported by EPA and available to users through the Center for Water Quality Modeling (CWQM). The code has been restructured to be compatible with the IBM PC. A companion program for converting SEMCOG formatted input data files to QUAL2E format is also available from CWQM.

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Table 1. Major Enhancements to QUAL-2 Code

(1) Algal, Nitrogen, Phosphorus Interactions

- organic nitrogen state variable
- organic phosphorus state variable

(2) Algal Growth Rate

- growth rate dependent upon both NH_3 and NO_3 concentrations
- preference factor input for NH_3
- algal self-shading
- three light functions for growth rate attenuation
- three growth rate attenuation options
- four diurnal averaging options for light

(3) Dissolved Oxygen

- new standard methods D.O. saturation function
- traditional SOD units (gm/m^2-day)
- dam reaeration option
- inhibition of nitrification at low D.O.

(4) Temperature

- linked to algal growth via solar radiation
- default temperature correction (θ) factors

(5) Arbitrary Non-Conservative Constituent

- first order decay
- removal (settling) term
- benthal source term

(6) Hydraulics

- input factor for longitudinal dispersion
- test for negative flow (i.e., withdrawal greater than flow)
- capability for incremental outflow along a reach

(7) Downstream Boundary

- option for specifying downstream boundary water quality constituent concentrations

(8) Input/Output Modifications

- detailed summary of hydraulic calculations
- new coding forms
- local climatological data echo printed
- enhanced steady state convergence summary
- five part final summary including plot of D.O. and BOD and components of the D.O. deficit

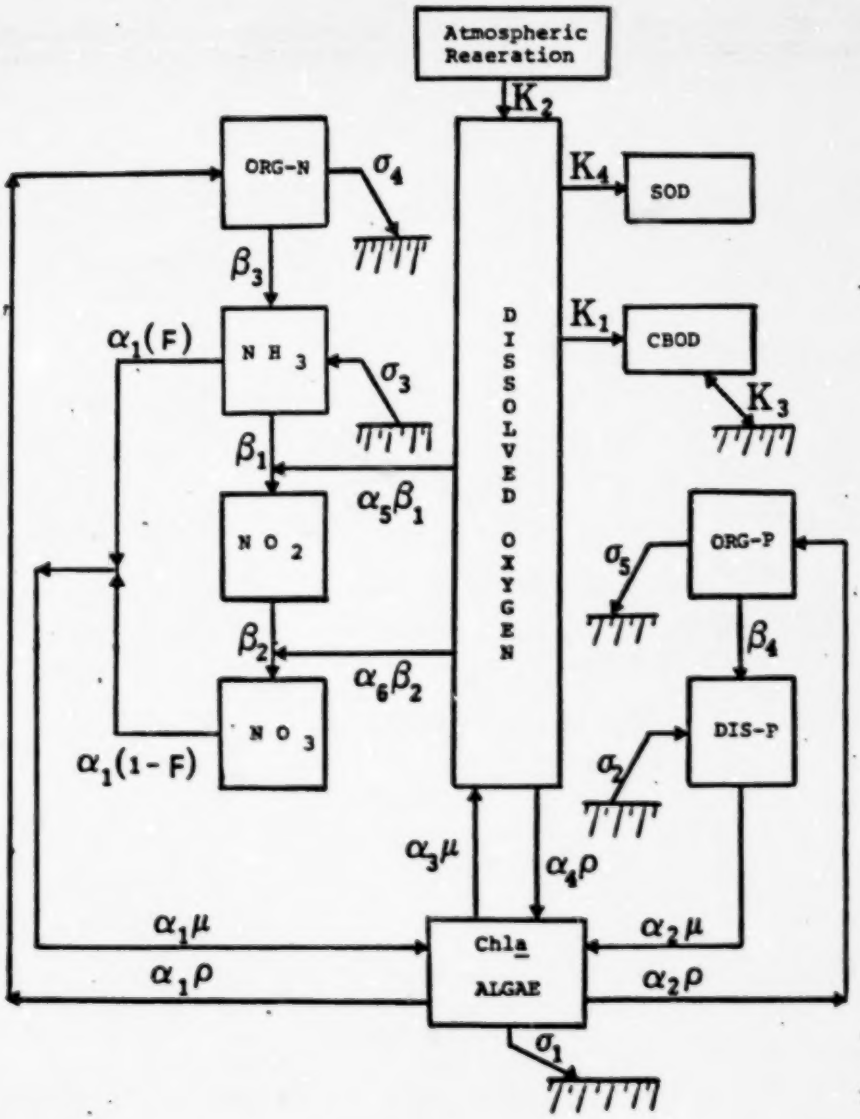

Figure 1. Major Constituent Relationships in QUAL2E